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Strategies for Single-Point Diamond Machining a Large Format Germanium Blazed Immersion Grating

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ABSTRACT

A large format germanium immersion grating was flycut with a single-point diamond tool on the Precision Engineering Research Lathe (PERL) at the Lawrence Livermore National Laboratory (LLNL) in November – December 2015. The grating, referred to as 002u, has an area of 59 mm x 67 mm (along-groove and cross-groove directions), line pitch of 88 line/mm, and blaze angle of 32 degree. Based on total groove length, the 002u grating is five times larger than the previous largest grating (ZnSe) cut on PERL, and forty-five times larger than the previous largest germanium grating cut on PERL. The key risks associated with cutting the 002u grating were tool wear and keeping the PERL machine running uninterrupted in a stable machining environment. This paper presents the strategies employed to mitigate these risks, introduces pre-machining of the as-etched grating substrate to produce a smooth, flat, damage-free surface into which the grooves are cut, and reports on trade-offs that drove decisions and experimental results.

Keywords: diffraction grating, immersion, germanium, diamond machining, diamond turning, subsurface damage

1. INTRODUCTION

The 002u grating has a total groove length of 350 m which required twenty-eight continuous days to cut using PERL. The previous largest grating produced by flycutting on PERL, based on total groove length, is a zinc selenide grating for the WINERED spectrometer, which has a total groove length of 63 m and took nine days to cut[1,2]. The previous largest germanium gratings cut on PERL are grisms for the LMIRcam Fizeau imager, which have a total groove length of 7.8 m and took one day to cut[3]. Comparing gratings by total groove length instead of area accounts for line density and provides a comparison basis for issues like tool wear and cutting days required.

The 002u grating benefits from previous work at LLNL using the PERL diamond turning machine in a flycutting configuration to produce blazed immersion gratings in infrared optical materials[1-7]. Additional insight for single-point diamond machining brittle materials was gleaned from earlier research at LLNL on diamond turning crystalline optics[8]. Summarizing the guidance from those earlier experiences, producing a smooth blaze face free of chipping at the groove edges requires pre-removal of any damaged substrate material, a sharp tool edge, a shallow enough depth of cut, not too fast of a feed rate in the along-groove direction, adequate cutting fluid for lubricating and cooling the tool tip, and the absence of contaminant particles that could damage the diamond tool.

2. BACKGROUND

2.1 Blazed immersed gratings

The immersed grating approach, especially when using a high index of refraction substrate, provides a more compact grating diffraction geometry than is obtainable when approaching the grooves from air or vacuum. In addition the entry and exit faces of the grating substrate provide refracting surfaces for controlling optical performance. With the appropriate blaze angle, the flat-faceted, saw-tooth shaped groove profile of a blazed grating provides the highest diffraction efficiency at the wavelength of interest. The grating geometry depends on the design of the overall optical system the grating is used in, and can be optimized during trade-offs among all the optical components. Grating grooves can be produced by chemical etching – if the substrate lends itself to etching – or by single-point diamond machining.

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Chemical etching can produce a flat blaze face if the groove geometry is aligned to the substrate crystallographic axes[9-12]. Single-point diamond machining can produce flat blaze faces even when the groove geometry is not aligned to the crystallographic axes, as is the case for the 002u grating, providing increased design freedom for the optical system.

2.2 Flycutting a grating

Figure 1 shows the PERL machine configured to flycut a grating. A single-point diamond tool is swung in a circular arc by a flycutter attached to a spindle, and the grating substrate is carried by a carriage back and forth in the along-groove direction. The height of the substrate is set so that the tool engages the substrate with a desired maximum depth of cut. The flycutter completes many revolutions while the grating substrate passes entirely underneath it. The along-groove feed rate determines how much material is removed during each flycutter revolution. If that feed rate is too fast, material removal is too aggressive and the grating groove profile becomes chipped and unusable. Experience cutting germanium gratings at LLNL showed that 10 mm/min was that limit, and small test gratings cut with the 002u grating tool showed that feed rate to be acceptable. After completing a groove, the flycutter is indexed in the cross-groove feed direction by the desired distance between grooves.

The next groove is cut in one of two ways: (1) bidirectional cutting, where the substrate is traveling in the opposite sense in the along-groove direction compared to the previous groove; or (2) uni-directional cutting, where the flycutter is fully retracted in the cross-groove feed direction so that it does not engage the substrate during the return stroke of substrate (which can be faster than the feed rate while cutting a groove) and then positioned for cutting the next groove while the substrate travels in the same direction as for the previous groove. Using the nomenclature of milling machines, bi-directional cutting involves alternate conventional and climb cutting, while unidirectional cutting is either conventional or climb cutting depending on the direction chosen for cutting the grating.

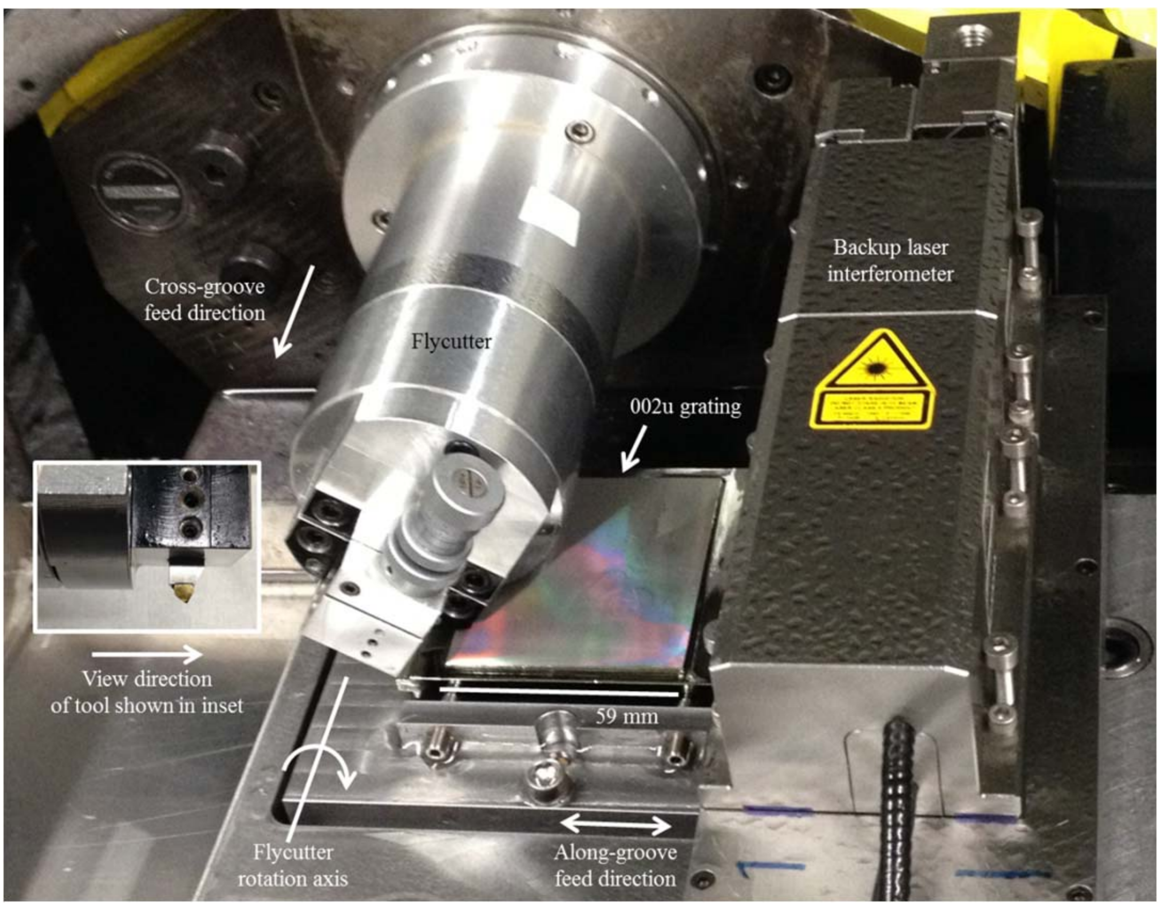

Figure 1. The 002u grating on the PERL machine, just after completing the 28-day grating cut.

3. KEY RISKS, MITIGATIONS, AND TRADE-OFFS

Many of the challenges faced when producing a blazed immersion grating by single-point diamond flycutting are already reported in the literature[1-7]. The 002u grating presented additional challenges by virtue of its size and steep blaze angle compared to earlier gratings produced at LLNL. Table 1 summarizes the key unique risks identified for the 002u grating and the trade-offs that were considered while determining how to mitigate those risks.

Table 1. Key risks, mitigations, and trade-offs for cutting the 002u grating.

		Risk addressed	
Mitigation	**Trade-off**	Tool wear	Keeping PERL running and a stable environment
Pre-machine substrate	Explore new process versus hitting a limit on tool wear and groove quality	✓	
Reduce total groove area	Shorter total groove length versus tightened position tolerances in the optical system	✓	✓
Bi-directional cutting	Possible groove quality and spectral ghosts versus 40% longer time for unidirectional cutting		✓
PERL backup systems	Adding and testing backup systems versus constrained schedule and budget		✓

3.1 Tool wear

Producing a successful grating by diamond flycutting involves producing one or more test gratings to determine if a sharp enough diamond tool is being used and to adjust (as needed) the blaze angle that is produced. Once a “good” tool is identified it can be used to produce gratings until it becomes too worn or damaged to produce grooves with crisp edges and smooth blaze faces. The total groove length of the 002u grating is forty-five times longer than the previous largest germanium grating cut at LLNL[3], so cutting 002u was equivalent to expecting a diamond tool to cut forty-five of the previously largest gratings – without re-sharpening between gratings – with no appreciable degradation in groove quality.

Reducing the total volume of material to be removed by the groove cutting tool reduces tool wear and lowers the likelihood of tool damage from an unintended hard inclusion in the grating substrate. This reduction was accomplished for the 002u grating by reducing the total grating area and pre-machining the substrate. Pre-machining the substrate allows using a shallower depth of cut over the entire grating aperture when flycutting the grooves, and is discussed in detail in the next section.

Reducing the total groove area set by the original grating design was seen as low-lying fruit for both decreasing tool wear and reducing the time needed for cutting the grooves uninterrupted in a stable environment. The original specified grating surface had been set at 76 mm x 76 mm (along-groove and cross-groove directions) based on certain assumptions for accommodating expected position tolerances when coating the grating and assembling it into an optical system. We explored this trade-space and settled on a balance that set the size of the grating surface to be 1 mm larger (per side) than the required grating clear aperture, which provided reasonable positioning tolerances while reducing the total groove length from 510 m in the original design to 350 m in the final design. This provided a 30% reduction in the total groove length to be cut by the tool. Taking into account the required along-groove over-travel of 5 mm needed on both sides of the substrate to clear the flycutter when indexing the PERL cross-groove carriage, and the 1 mm increase in cross-groove length added to the CNC program to accommodate setup error, the original design would have taken 40 days to cut (bi-directional). The reduced groove area for the final design reduced the cutting time by 30% to 28 days.

3.2 Bi-directional versus unidirectional cutting

Taking into account the feed rate limits of the PERL machine, unidirectional cutting of a grating requires 40% more time than bi-directional cutting, so if all other things are equal bi-directional cutting is preferred. Two potential issues with bi-directional cutting had to be considered: (1) the quality of grooves produced by conventional cutting and by climb cutting; and (2) possible spectral ghosts due to odd versus even numbered grooves being offset from each other because of the finite transverse shift in the along-groove feed carriage when it changes directions. Both of these potential issues were explored while cutting the test gratings that preceded the 002u grating. Groove quality was equally good for conventional and climb cut grooves, and spectral ghosts from bi-directionally cut grooves were acceptable for the intended use of the grating. Having mitigated the risks associated with bi-directional cutting enabled confidently using it to fabricate the 002u grating with a 28-day cut instead of the 40% longer 39-day cut that unidirectional cutting would have taken for the same sized grating.

3.3 Keeping PERL running and a stable environment

Ensuring that the PERL machine would run uninterrupted in a stable environment for twenty-eight days presented many technical and logistical challenges. PERL was designed and built more than thirty years ago[13], most of the subsystems are unique and/or outdated, full recovery from unexpected stoppages is not always possible, and temperature stability for the machine depends on a chain of systems outside of PERL that present multiple single-point failure scenarios.

PERL is equipped with an emergency stop system intended to protect personnel and the machine in case of certain failures, such as a loss of position feedback on the along-groove or cross-groove direction carriages, or a drop in air pressure to the air bearing spindle that supports the flycutter. During the period leading up to cutting the 002u grating, emergency stops were occurring without warning so we had to either adapt to them or engage in a prolonged investigation of the causes and remedy them. Schedule and budget constraints associated with producing the 002u grating dictated pursuing the former route.

During an emergency stop the PERL carriages shift slightly and their position data is lost, so grooves cut after restarting the machine would be offset from the grooves cut before the stop. This problem was addressed for the 002u grating by a relatively straight forward method. Referring to Figure 1, a backup metrology-grade displacement-measuring interferometer was temporarily added to PERL. The backup laser provided a second measurement of the cross-groove infeed position of the flycutter. Powering the backup laser through a dedicated uninterruptable power supply (UPS) and recording the measured displacement provided a robust record of the cross-groove feed carriage position, which would allow repositioning the carriage relative to the last known good groove before an emergency stop within an acceptable tolerance.

A lesson learned while cutting the WINERED grating[1] was that a temporary reduction in voltage supplied to the facility housing PERL (electrical brown-out) could cause an emergency stop. In the case of the WINERED grating, a planned 14-day grating cut was reduced to a 9-day cut by such an event because there was no means to confidently position additional grooves after restarting the machine. For the 002u grating, rather than only depend on the backup laser to recover from an emergency stop, we sought to better avoid a brown-out induced emergency stop by adding an UPS system to the PERL motor drivers to complement the UPS already present for the PERL control computer. During the 28-day cut of the 002u grating the PERL machine did not experience an emergency stop.

Maintaining a stable environment while cutting the 002u grating required continuous coordination with ongoing work on other facility systems that could potentially affect PERL, and dealing with failures in facility heating and cooling systems that the PERL temperature stability depends on. On the 22nd day of the 28-day cut a boiler that provides hot water for the room temperature control system failed, but it was discovered and repaired before significantly affecting the PERL temperatures of concern: room air outside the PERL enclosure, air inside the enclosure, machine, and spindle. On the 24th day a chiller that provides cold water for the room temperature control system failed and prompted us to suspend indexing the flycutter until the chiller was repaired and temperature stability was restored.

4. PRE-MACHINING THE GRATING SUBSTRATE

Before cutting grooves, the surface of the grating substrate is prepared by removing potentially damaged substrate material from previous processing steps and ensuring there are no contaminant particles that could damage the diamond tool used to cut the grooves. If the surface of the substrate is not damage-free the groove cutting tool can cause excessive tear-out of material resulting in unacceptable groove profile quality. Since the groove cutting tool will eventually encounter every square micrometer of the substrate surface, at a depth up to 100 micrometers, if an unintended hard particle – like a piece of grit from a grinding or lapping process – is present in that volume of material the tool will find it, become damaged, and then produce degraded grooves.

As with previous gratings cut in infrared optical materials at LLNL, the 002u grating substrate was chemically etched to remove an approximately 100 micrometer thick layer of material. Figure 2a shows the surface of the 002u substrate after etching, which was measured to have a 50 micrometer PV height variation over the entire surface and 15 micrometer PV waviness over shorter distances. If grooves were cut in the as-etched surface the depth of cut would vary by at least 50 micrometer over the entire surface, with abrupt changes that could result in damaged grooves, so reducing the surface height variation of the as-etched grating substrate is advantageous. This was accomplished for the 002u grating by pre-machining the as-etched substrate using the PERL machine in a conventional turning configuration to spiral-cut the surface. Figure 2b shows the completed pre-machined substrate surface, which has a measured surface figure of 0.7 micrometer PV for the entire surface, and a measured surface roughness of 4 nanometer Ra (arithmetic average roughness) over a 0.176 mm x 0.235 mm patch.

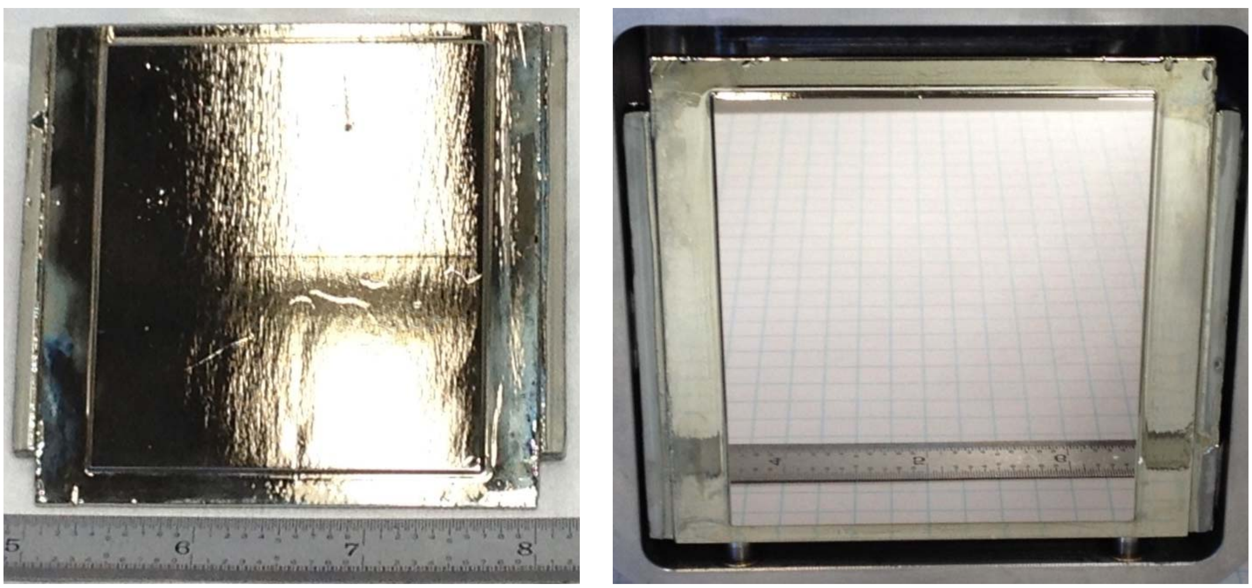

Figure 2. (a, left) As-etched surface of the 002u grating substrate; (b, right) pre-machined 002u grating substrate.

Table 2. Taper-down sequence of cuts and cutting parameters used to pre-machine the 002u grating substrate.

Number of passes	Depth of cut (micrometer)	Cross-feed rate (mm/min)	Spindle speed: 500 RPM
12x	5	2.5	Tool rake angle: -15 degree
1x	2.5	0.25	Tool nose radius: 0.25 mm
1x	1.3	0.13	Coolant: odorless mineral oil mist spray (paraffin-based)
1x	0.6	0.13	

Table 2 shows the cutting parameters and taper-down sequence of cuts used to pre-machine the 002 grating substrate. A similar taper-down sequence for single-point machining a brittle material is described in [8]. The intent of a taper down sequence is to remove the subsurface damage produced by the previous cut while not creating more new subsurface damage than can be removed by the following cut, culminating in a final cut that is thin enough for material removal to be in the ductile regime rather than the brittle regime.

Referring to Figure 3, during pre-machining the as-etched 002u substrate was mounted to the PERL spindle via a fixture that provides two-plane balancing of the wedged substrate and holds the substrate the same way the grating is mounted in the optical system it was designed for.

The relationship between the groove cutting tool and grating substrate is shown in Figure 4. Referring to the view along the grooves, after a groove is fully completed in the along-groove direction (out of the page) the grating groove tool is indexed to the left and then the next groove is formed. The view across the grooves illustrates the successive sweeps of the tool tip through the substrate as the flycutter carrying the tool rotates and the substrate moves under it in the along-groove direction. When flycutting in this configuration the varying chip thickness during each sweep of the tool tip through the workpiece creates a taper-down cut when moving in the climb milling direction, and a taper-up cut when moving in the conventional milling direction.

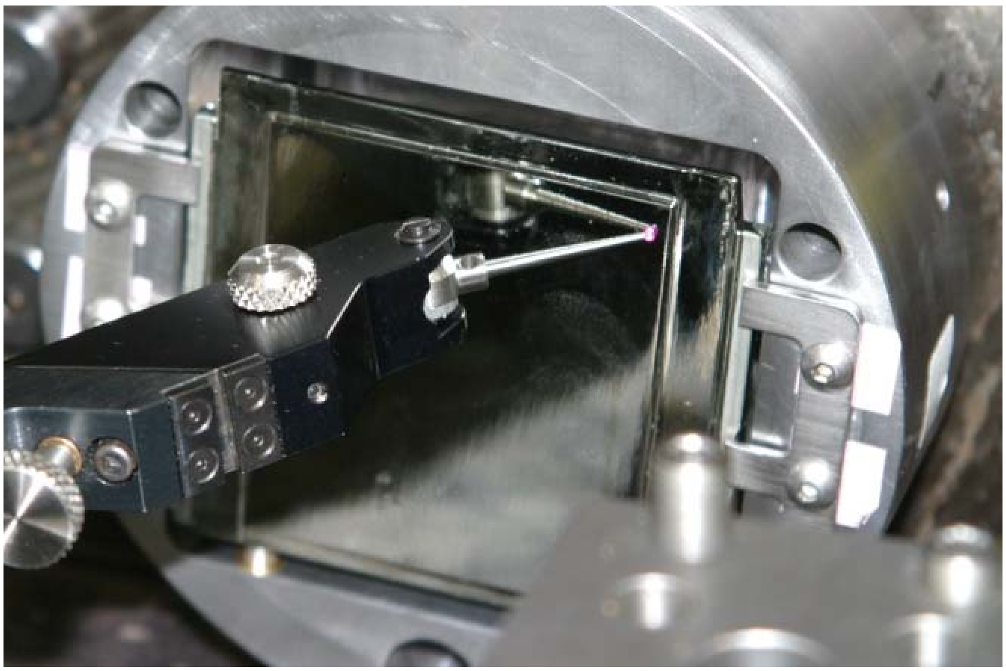

Figure 3. As-etched grating 002u substrate mounted to the PERL spindle in preparation for pre-machining by a tool (not visible) mounted to the tool-holder in the lower-right foreground. The finger-type LVDT gauge is used to find the high point in preparation for the taper-down sequence of spiral cuts.

The determination of the depth of cut shown in Figure 4 takes into account the nominal groove depth, the error in setting the height of the grating substrate under the flycutter (tool height), the non-flatness of the substrate, and the error in leveling the substrate under the flycutter. A strategy for removing the leveling error term is suggested in future work.

The order-of-magnitude analysis shown in Figure 4 indicates that pre-machining the as-etched 002u substrate before cutting the grooves provided a 35% reduction in the total length of engagement between the grating groove tool tip and germanium, and a 60% reduction in the volume of germanium removed by the groove cutting tool. Both of these factors reduce tool wear. Moreover, by pre-machining the substrate the expected depth of cut variation during groove formation was reduced from a range of 15 – 70 micrometer to a range of 15 – 17 micrometer across the entire grating surface, reducing the likelihood of damaged grooves due to large (and possibly abrupt) changes in uncut material chip thickness.

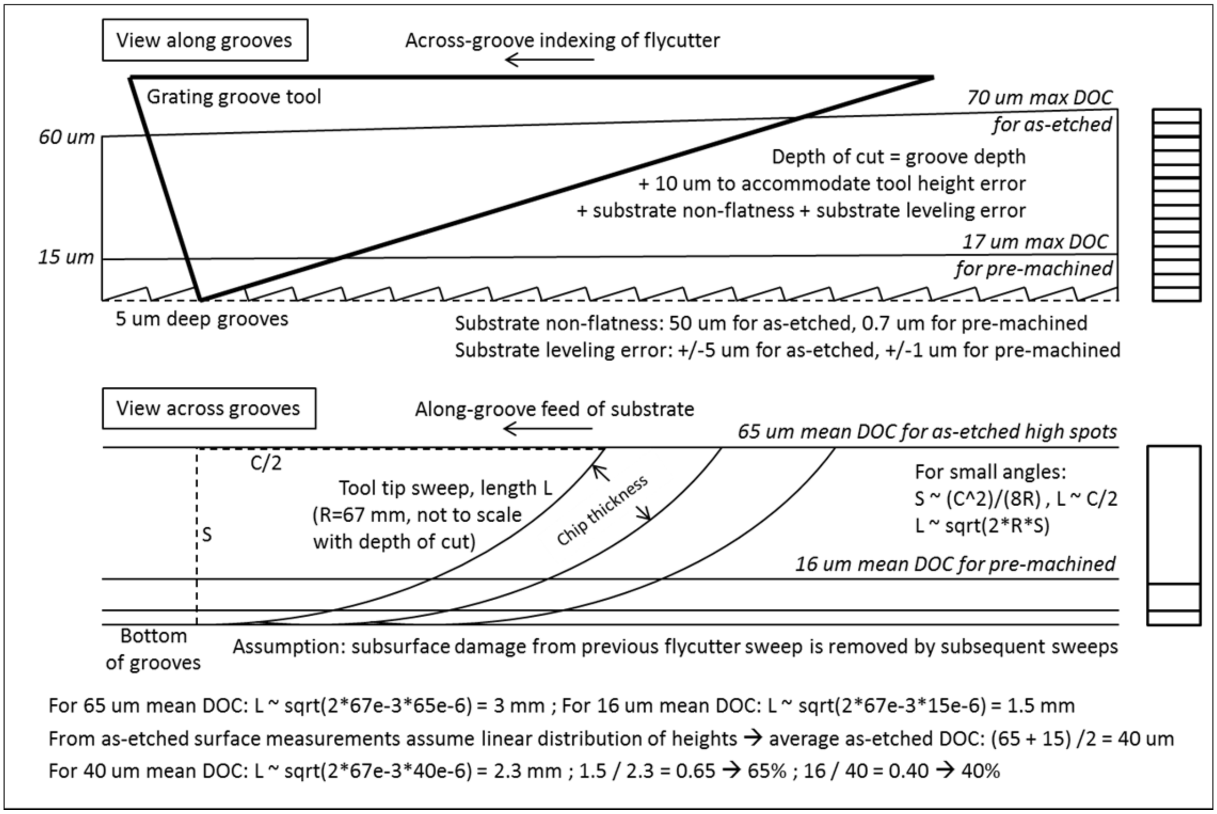

Figure 4. Relationship between the tip of the groove cutting tool (carried by the flycutter) and the grating substrate. Values are for the as-etched and pre-machined 002u grating substrate. View along the grooves is in the opposite direction of the view of the tool shown in Figure 1.

5. GRATING 002U

Before cutting the 002u grating an accelerated test program was conducted using small (9 mm x 10 mm) germanium substrates to determine the cutting parameters shown in Table 3, and to identify a sharp enough diamond tool. Conducting cutting tests on substrates with a known history allows controlling variables that could affect the outcome.

Table 3. Cutting parameters used to produce the 002u grating grooves.

Spindle speed: 1000 RPM	Flycutter swing radius: 33 mm
Along-groove feed rate: 10 mm/min, alternating conventional and climb milling	
Cross-groove indexing: away from blaze face (see Figure 4)	
Tool tip included angle: 90 degree (between blaze face and adjacent face)	
Tool rake angle: -30 degree (symmetric with bisector of included angle)	
Tool nose radius: “sharp tip” (best effort by tool vendor)	
Nominal groove depth: 5 micrometer	
Depth of cut: 15 – 17 micrometer (normal to grating surface, see Figure 4)	
Coolant: odorless mineral oil mist spray (paraffin-based)	

Groove cutting on the 002u grating began 16 November 2015 and continued for twenty-eight continuous days until the entire grating surface was completed on 14 December. Figure 5 shows the 002u grating just after completing the 28-day cut. Groove quality, depicted in Figure 6, is good across the entire grating surface and met the requirements for the grating.

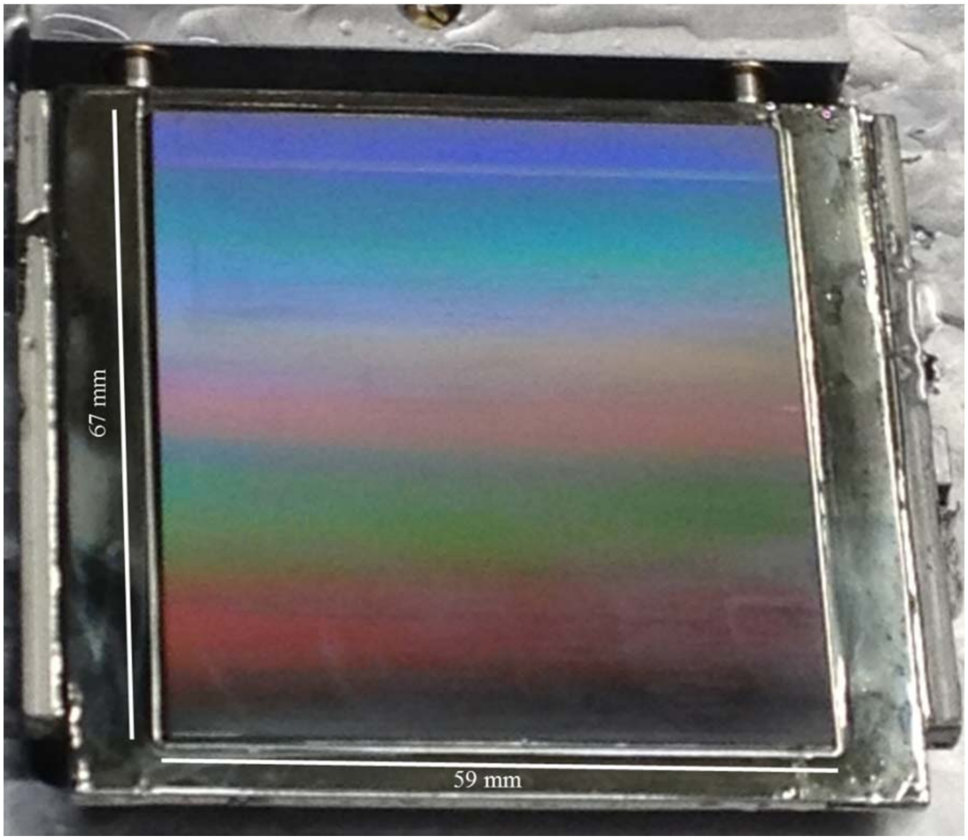

Figure 5. The 002u grating, just after completing the 28-day cut and in the fixture used to mount it to the PERL machine. The slight change in the diffracted light gradient near the top of the image corresponds to the chiller failure on day 24.

Measurement of the 002u grating diffracted beam wavefront quality was obtained with a Fizeau interferometer externally illuminating the full ruled surface at 633 nanometer. The resulting wavefront map is shown in Figure 7. Taking into account the elliptical beam footprint on the grating when used in the optical system it was designed for, the diffracted wavefront is 1.2 wave PV and 0.33 wave RMS, which was acceptable. The mid spatial frequency waviness in the cross-groove direction is likely due to changes in atmospheric pressure and temperature while cutting the grooves, both of which affect the absolute length of the laser interferometers used by the PERL machine for position feedback, and the later affecting length changes in the PERL structural loop (which includes the workpiece and tool).

The blaze angle of the 002u grating was measured by externally illuminating the grooves with a 633 nanometer laser and comparing the distribution of energy in the diffracted orders to a prediction based on scalar diffraction theory, as described in [6]. The measured blaze angle is within 0.03 degree of the target value, which is well within the tolerance of +/- 0.15 degree set for the grating, and the measured diffraction efficiency of the grooves was acceptable.

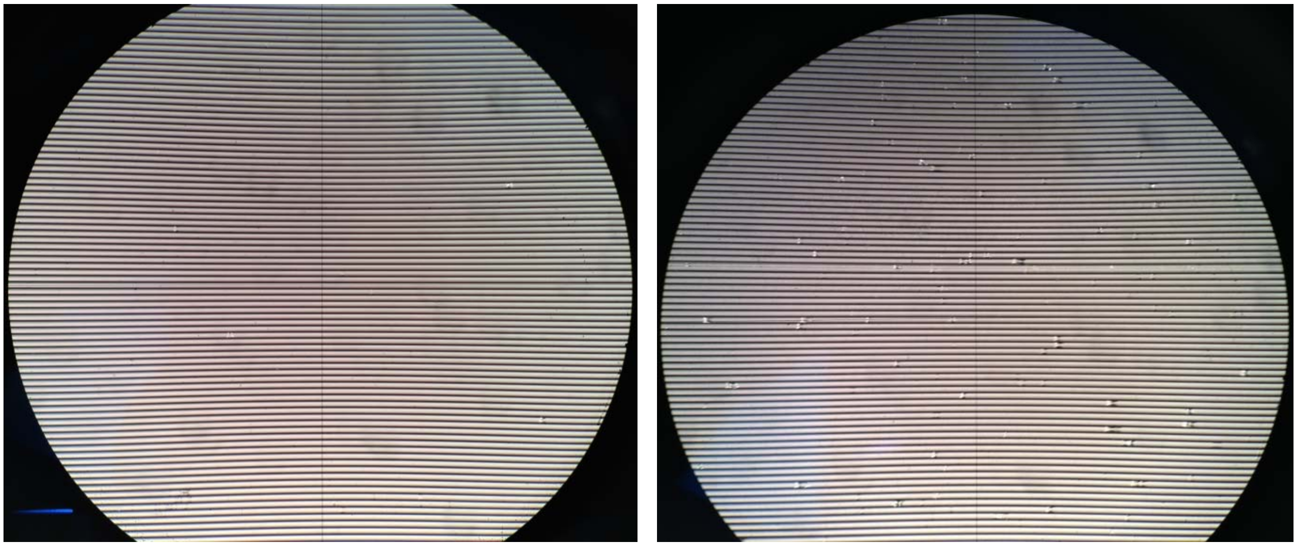

Figure 6. Optical microscope images of the 002u grating grooves at 200x magnification showing grooves formed near the beginning (left) and near the end (right) of the 28-day cut. Slight (acceptable) chipping appear as small breaks in the lines. What appears to be a missing groove in the image on the right is actually a shallow groove associated with the chiller failure on day 24. The apparent non-straightness of the grooves is an artifact of the camera used to record the images.

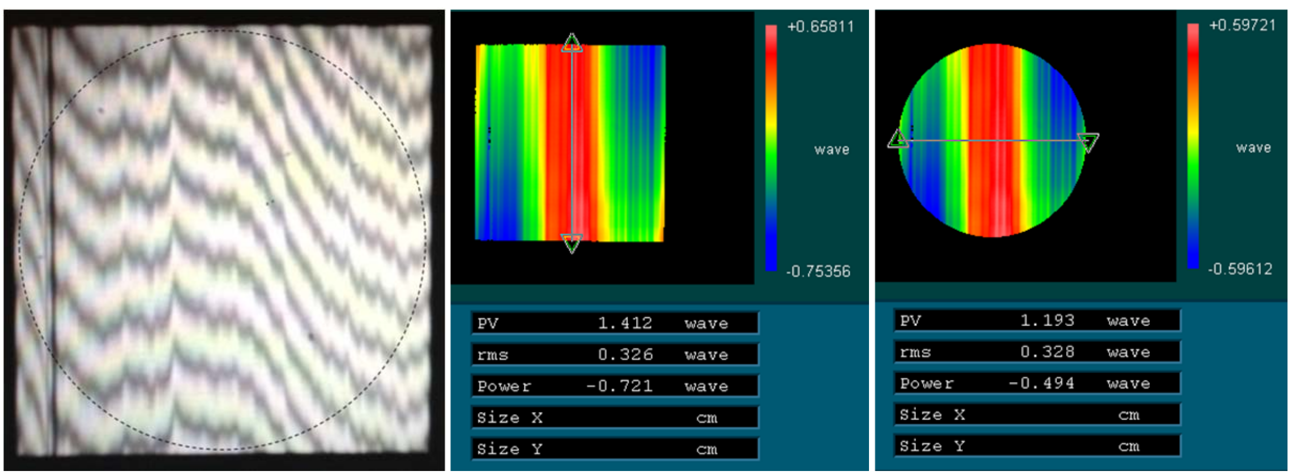

Figure 7. Full aperture (59 mm x 67 mm) Fizeau interferometer measurement of the 002u grating diffracted beam wavefront quality, externally illuminated at 633 nanometer. In these images the grooves were cut from right to left. The ellipse represents the approximate beam footprint on the grating when installed in the optical system it was designed for. For the area enclosed by the ellipse the diffracted wavefront is 1.2 wave PV and 0.33 wave RMS.

6. SUMMARY

A large format germanium immersion grating was flycut with a single-point diamond tool on the Precision Engineering Research Lathe (PERL) at the Lawrence Livermore National Laboratory (LLNL) in November – December 2015. Referred to as 002u, the grating took 28 continuous days to cut, and based on total groove length is 5x larger than the previous largest grating (ZnSe) cut on PERL and 45x larger than the previous largest germanium grating cut on PERL.

Many of the challenges faced when producing a blazed immersion grating by single-point diamond flycutting are already reported in the literature. The 002u grating presented additional challenges by virtue of its size compared to earlier gratings produced at LLNL, specifically tool wear and the challenge of keeping the PERL machine running and in a stable environment for such a long time.

Four key risk mitigations were employed for the 002u grating. (1) Reducing the total grating area by tightening the positioning tolerances for the grating in the optical system it was designed for. (2) An accelerated test program to prove that bi-directional groove cutting was acceptable, and that pre-machining the grating substrate was viable. (3) Pre-machining the as-etched grating substrate to reduce the total length of engagement between the grating groove tool tip and germanium by 35%, and reduce the volume of germanium removed by the groove cutting tool by 60%. (4) Adding a backup metrology laser to the PERL cross-groove indexing carriage to allow recovery from an emergency stop and adding uninterruptable power supplies to avoid an emergency stop due to possible dips in supply voltage to the machine. Mitigations (1) and (2) enabled cutting the 002u grating in 28 days instead of 56 days, (3) and (4) helped prevent surprises, and (3) leads to suggested future work.

7. FUTURE WORK

The 002u grating demonstrates that good quality grooves can be cut into a pre-machined germanium substrate with a single-point diamond tool. Pre-machining of other infrared optical materials may also be viable and could be proven by straightforward tests; the cutting parameters described in this paper provide a starting point for those tests.

By pre-machining the as-etched substrate the depth of cut during groove formation was reduced from a range of 15 – 70 to 15 – 17 micrometer. This reduction in depth of cut variation across the entire surface of the grating may enable using a faster along-groove feed rate than the accepted limit of 10 mm/min established for cutting grooves in as-etched germanium substrates. The schedule for the 002u grating did not allow explore this possibility, but future work on other gratings might.

A natural extension of the work presented in this paper is to combine the fixture used to hold the grating substrate during pre-machining with the fixture used to hold the substrate when flycutting the grooves. By using a single fixture for both machining operations, and leaving the substrate attached to it, the substrate leveling error described in Figure 4 can be mitigated. When the grating surface is pre-machined by spiral-cutting on a diamond turning machine the freshly created flat surface will be parallel to the back of the fixture to better than 1 micrometer. When the common fixture is moved to the along-groove carriage for cutting the grooves the pre-machined surface will already be parallel to the along-groove carriage travel. Ensuring that the pre-machined surface is parallel to the cross-groove indexing carriage travel is a function of how well the machine is set up.

If a pre-machined substrate is accurately aligned to the flycutting machine’s travel axes the depth of cut of the groove cutting tool can be adjusted to form flat-tipped grooves, retaining the pre-machined surface for the flat tips. When used in immersion, the tip of the grating groove is in a shadowed area, as shown in [9], so the width of that shadow would define the allowable width of the flat tip. Flat-tipped grooves may be less prone to chipping during the groove formation process and could prove to be more durable.

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